Bath generated work extraction in two-level systems

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Abstract. The spin-boson model, often used in NMR and ESR physics, quantum optics and spintronics, is considered in a solvable limit to model a spin one-half particle interacting with a bosonic thermal bath. By applying external pulses to a non-equilibrium initial state of the spin, work can be extracted from the thermalized bath. It occurs on the timescale $\mathcal{T}_2$ inherent to transversal ('quantum') fluctuations. The work (partly) arises from heat given off by the surrounding bath, while the spin entropy remains constant during a pulse. This presents a violation of the Clausius inequality and the Thomson formulation of the second law (cycles cost work) for the two-level system.

Introduction. After E.L. Hahn discovered the spin-echo in NMR physics [1], it was soon considered to be a counterexample for irreversibility and for the second law [1, 2]; for a recent discussion see e.g. [2, 3]. In the present contribution we will show in a different context that NMR-physics contains quantum effects which should be interpreted as limits of the second law [4]. Within the same general program we recently analyzed the thermodynamics of the Caldeira-Leggett model for a quantum harmonic oscillator coupled to a thermal bath [5]. At low temperatures various formulations of the second law are violated: the Clausius inequality $\bar{d}\mathcal{Q} \leq T\mathrm{d}S$ is broken, the rates of energy dispersion and entropy production can be negative, and certain cycles are possible where heat extracted from the bath is fully converted into work ("perpetuum mobile"). The present analysis of the spin-boson model reveals a different quantum mechanism limiting the validity of the second law.

The Hamiltonian of the problem reads:

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}(\Delta) = \mathcal{H}_S + \mathcal{H}_B + \mathcal{H}_I, \qquad (1)\\
\mathcal{H}_S &= \frac{\varepsilon}{2}\hat{\sigma}_z + \frac{\Delta(t)}{2}\hat{\sigma}_x, \quad \mathcal{H}_B = \sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k, \quad \mathcal{H}_I = \frac{1}{2}\sum_k g_k(\hat{a}_k^\dagger + \hat{a}_k)\hat{\sigma}_z.
\end{aligned}$$

This is a spin-$\frac{1}{2}$ interacting with a bath of harmonic oscillators (spin-boson model [7, 8]); $\mathcal{H}_S$, $\mathcal{H}_B$ and $\mathcal{H}_I$ stand for the Hamiltonians of the spin, the bath and their interaction, respectively. $\hat{\sigma}_x$, $\hat{\sigma}_y$ and $\hat{\sigma}_z = -i\hat{\sigma}_x\hat{\sigma}_y$ are Pauli matrices, and $\hat{a}_k^\dagger$ and $\hat{a}_k$ are the creation and annihilation operators of the bath oscillator with the index k, while the g_k are the coupling constants. For an electron in a magnetic field B, $\varepsilon = \bar{g}\mu_B B$ is the energy, with $\bar{g}$ the gyro-magnetic factor and μ_B the Bohr magneton. We shall consider a situation where $\Delta(t) = 0$ for almost all times. This is a prototype of a variety of physical systems [7], and

known to be exactly solvable [7, 8], since the z-component of the spin is conserved, and with it the spin energy. Physically it means that we restrict ourselves to times much less than $\mathscr{T}_1$ (relaxation time of $\hat{\sigma}_z$). In ESR physics [9] the model represents an electron-spin interacting with a bath of phonons, for NMR it can represent a nuclear spin interacting with a spin bath, since in certain natural limits the latter can be mapped to the oscillator bath. In quantum optics it is suitable for describing a two-level atom interacting with a photonic bath [10].

Starting from general physical arguments [7], one typically takes the quasi-Ohmic spectral density of the bath $J(\omega) = \sum_k g_k^2 \delta(\omega_k - \omega)/(\hbar\omega_k) = g\hbar \exp(-\omega/\Gamma)/\pi$, where g is the dimensionless damping constant and the exponential cuts off the coupling at $\omega \gg \Gamma$, the maximal frequency of the bath. As usual, the thermodynamic limit for the bath has been taken here.

Since $\Delta = 0$, one has conservation of $\hat{\sigma}_z(t) = \hat{\sigma}_z(0)$ (in the Heisenberg picture). Due to this one has [4]:

$$\sum_k g_k [\hat{a}_k^\dagger(t) + \hat{a}_k(t)] = \hat{\eta}(t) - \hat{\sigma}_z G(t), \tag{2}$$

$$\hat{\eta}(t) \;=\; \sum_k g_k [\hat{a}_k^\dagger(0) e^{i\omega_k t} + \hat{a}_k(0) e^{-i\omega_k t}], \qquad G(t) = g\frac{\hbar\Gamma}{\pi}\frac{\Gamma^2 t^2}{1+\Gamma^2 t^2},$$

where $\hat{\eta}(t)$ is the quantum noise operator, and where the structure of $G(t)$ shows that $1/\Gamma$ is the relaxation time of the bath.

Separated initial state. To describe situations, where the spin was suddenly brought into the contact with the bath, e.g. an electron injected into semiconductor, atom injected into a cavity, or exciton created by external radiation, we make the assumption that initially, at $t = 0$, the spin and the bath are in a separated state, the latter being Gibbsian at temperature $T = 1/\beta$: $\rho(0) = \rho_S(0) \otimes \exp(-\beta \mathscr{H}_B)/Z_B$, where $\rho_S(0)$ is the initial density matrix of the spin. In this situation the quantum noise is stationary and Gaussian with average zero. The Heisenberg equation $\hbar\dot{\hat{\sigma}}_\pm = i\,[\pm\varepsilon + \hat{\eta}(t) - G(t)]\,\hat{\sigma}_\pm$ for $\hat{\sigma}_\pm = \hat{\sigma}_x \pm i\,\hat{\sigma}_y$ can be solved exactly with the result [4]:

$$\langle \hat{\sigma}_\pm(t)\rangle = e^{\pm i\omega_0 t - \xi(t)} \langle \hat{\sigma}_\pm(0)\rangle, \quad \xi(t) = \frac{g}{\pi} \ln \frac{\Gamma^2\left(1+\frac{T}{\hbar\Gamma}\right)\,\sqrt{1+\Gamma^2 t^2}}{\Gamma\left(1+\frac{T}{\hbar\Gamma} - i\frac{Tt}{\hbar}\right)\Gamma\left(1+\frac{T}{\hbar\Gamma} + i\frac{Tt}{\hbar}\right)}, \tag{3}$$

where $\langle \hat{\eta}(t)\hat{\eta}(0) + \hat{\eta}(0)\hat{\eta}(t)\rangle = 2\hbar^2\ddot{\xi}(t)$, $\omega_0 = \varepsilon/\hbar$, and $\langle \hat{\sigma}_x(t)\rangle$, $\langle \hat{\sigma}_y(t)\rangle$ are determined via the real and imaginary part of $\langle \hat{\sigma}_\pm(t)\rangle$. For $t \gg 1/\Gamma$ (3) brings $\xi(t) \simeq t/\mathscr{T}_2$, $\mathscr{T}_2 = \hbar/(gT)$. $\mathscr{T}_2$ can thus be identified with the transversal decay time.

The density matrix of the spin reads $\rho_S = \frac{1}{2} + \frac{1}{2}\sum_{k=x,y,z} \langle \hat{\sigma}_k(t)\rangle\,\hat{\sigma}_k$. Its von Neumann entropy equals $S_{\mathrm{vN}} = -\mathrm{tr}\rho_S \ln \rho_S = -p_1 \ln p_1 - p_2 \ln p_2$, where $p_{1,2} = \frac{1}{2} \pm \frac{1}{2}|\langle \vec{\sigma}\rangle|$, $\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$. In the course of time $|\langle \vec{\sigma}(t)\rangle|$ decays to $|\langle \hat{\sigma}_z(0)\rangle|$, which makes the von Neumann entropy increase. Since there is no heat flow - the energy is conserved - this is in agreement with a formulation of the second law: the entropy of closed system, or of an open system without energy transfer (the spin in contact with the bath), cannot decrease.

A sudden pulse. So far we considered the Hamiltonian (1) with $\Delta = 0$. A fast rotation around the x-axis is described by taking $\Delta \neq 0$ during a short time δ_1; this is called a

fast pulse [9]. If $\Delta \sim 1/\delta_1$ is large, the evolution operator describing the pulse becomes $U_1 = \exp(-i\delta_1 \mathscr{H}(\Delta)/\hbar) \approx \exp(\frac{1}{2} i\,\theta \hat{\sigma}_x) + \mathscr{O}(\delta_1)$, where $\theta = -\delta_1 \Delta/\hbar$ is the rotation angle, $U_1^{-1}\,\hat{\sigma}_{y,z} U_1 = \hat{\sigma}_z \sin\theta \pm \hat{\sigma}_y \cos\theta$. During the sudden switchings of $\Delta(t)$ from 0 to Δ and from Δ to 0, the state of the system does not change, so $\rho(t+\delta_1) = U_1\,\rho(t)\,U_1^{-1}$. The work done by the source is the change of the total energy,

$$W_1(t) = \mathrm{tr}\left[\rho(t)(\mathscr{H}(\Delta) - \mathscr{H}) + \rho(t+\delta_1)(\mathscr{H} - \mathscr{H}(\Delta))\right] = \mathrm{tr}\,\rho(t)(U_1^{-1}\mathscr{H} U_1 - \mathscr{H}),$$

since $[U_1, \mathscr{H}(\Delta)] = 0$.

Our main interest is work extraction from the bath. In order to ensure that the pulse does not change the energy of the spin, we first consider the case $\varepsilon = 0$, where the spin has no energy. For small g, $\theta = -\pi/2$ and $t \gg 1/\Gamma$ the work appears to be

$$W_1 = \frac{g\hbar\Gamma}{2\pi} + \frac{gT}{2}\langle \hat{\sigma}_x(0)\rangle\, e^{-t/\mathscr{T}_2} \tag{4}$$

If for a fixed t, temperature is neither too large nor too small, $Te^{-t/\mathscr{T}_2} > \hbar\Gamma/\pi$, work can be extracted ($W_1 < 0$), provided the spin started in a coherent state $\langle \hat{\sigma}_x(0)\rangle = -1$. This possibility to *extract work* from the equilibrated bath ($t\Gamma \gg 1$) contradicts to the Thomson's formulation of the second law out of equilibrium. It disappears on the timescale $\mathscr{T}_2$, because then the spin looses its coherence, $\langle \hat{\sigma}_{x,y}(t)\rangle \to 0$. Notice that any combination of $\pm\pi$ pulses (this is a classical variation, since the coherence is not involved) can extract work only from a non-thermalized bath, i.e. for times $\sim 1/\Gamma$. Thus, the effect is indeed essentially quantum.

Initial preparation via a rotation. Our approach also allows to consider a specific, well controllable non-equilibrium initial state: a Gibbsian of the total system, $\rho_G = \exp(-\beta\mathscr{H})/Z$, in which at $t=0$ the spin is rotated ("zeroeth pulse") over an angle $-\frac{1}{2}\pi$ around the y-axis, $\rho(0) = U_0\,\rho_G\,U_0^{-1}$, with $U_0 = \exp(-i\pi\hat{\sigma}_y/4)$. This maps $\hat{\sigma}_x \to \hat{\sigma}_z$, $\hat{\sigma}_z \to -\hat{\sigma}_x$. Such a state models the optical excitation of the spin, as it is done in NMR and spintronics. Though $\rho(0)$ does not have the product form mentioned above (7), the problem remains exactly solvable. Taking $\theta = -\frac{1}{2}\pi$ one now gets

$$W_1 \approx \frac{g\hbar\Gamma}{2\pi} - \left[\frac{\varepsilon}{2}\sin\omega_0 t + \frac{gT}{2}\cos\omega_0 t\right]\tanh\frac{\beta\varepsilon}{2}\; e^{-t/\mathscr{T}_2} \tag{5}$$

where $\gamma(t) = (g/\pi)\arctan[\Gamma t]$ arises from friction, with $\gamma(\infty) = g/2$. Typically g is small, so work is extracted ($W_1 < 0$) when the sine function is positive. The work decomposes as $W_1 = \Delta U - \Delta Q$, into the change in spin energy due to the pulse, $\Delta U \simeq -(\varepsilon/2)\,\sin\omega_0 t\;\tanh[\beta\varepsilon/2]\,e^{-t/\mathscr{T}_2}$, and the heat absorbed from the bath

$$\Delta Q \approx \frac{g}{2}\left[-\frac{\hbar\Gamma}{\pi} + T\cos\omega_0 t\;\tanh\frac{\beta\varepsilon}{2}\,e^{-t/\mathscr{T}_2}\right] \tag{6}$$

Notice its similarity with $-W_1$ of Eq. (4). An interesting case is where work is performed by the total system ($W_1 < 0$) solely due to heat taken from the bath ($\Delta Q > 0$, $\Delta U = 0$). This process, possible by choosing $t \approx 2\pi n/\omega_0$ with integer n, can be considered as a

cycle of a perpetuum mobile, forbidden by folklore minded formulations of the second law. Indeed, under a rotation the length $|\langle\vec{\sigma}\rangle|$, and with it the von Neumann entropy, is left invariant, so one has a process with $\Delta Q > 0$, $\Delta S_{\rm vN} = 0$, which violates the Clausius inequality $\Delta Q \leq T\Delta S_{\rm vN}$. The work needed at time zero to rotate the spin is $W_0 = (\varepsilon/2)\tanh[\beta\varepsilon/2] + g\hbar\Gamma/(2\pi)$, representing the work done on the spin and on the bath, respectively. It can be verified that the total work $W_0 + W_1$ is always positive, so Thomson's formulation for a cyclic change [6] (here: the combination of the pulses at time $t = 0$ and t) starting from equilibrium is obeyed.

Two pulses in a rotated initial Gibbsian state. If there are many (very weakly interacting) spins, each in a slightly different external field, there appears an inhomogeneous broadening of the $\omega_0 = \varepsilon/\hbar$ line, for which we assume the distribution

$$p(\omega_0) = \frac{2}{\pi}\frac{[\mathcal{T}_2^*]^{-1}}{(\omega_0 - \bar{\omega}_0)^2 + [\mathcal{T}_2^*]^{-2}} \tag{7}$$

having average $\bar{\omega}_0$ and inverse width $\mathcal{T}_2^*$, typically much smaller than $\mathcal{T}_2$. In this case the gain for a single pulse is washed out, leaving only the loss $\Delta Q = -g\hbar\Gamma/2\pi$, so two pulses are needed. We consider again the rotated initial Gibbsian state, and perform a first $-\frac{1}{2}\pi$ pulse around the x-axis at time t_1 and a second $\frac{1}{2}\pi$ pulse at time $t_2 = t_1 + \tau$ (the standard $\frac{1}{2}\pi$, π combination would not expose an interesting role of the bath). In the regime of small g and large $t_1 \sim \mathcal{T}_2$ the work in the second pulse is

$$\begin{aligned} W_2 &= \frac{g\hbar\Gamma}{2\pi} - \frac{1}{2}e^{-t_1/\mathcal{T}_2}\varepsilon\sin\omega_0\tau\,\tanh\frac{\beta\varepsilon}{2} \\ &- \frac{1}{2}e^{-t_2/\mathcal{T}_2}\tanh\frac{\beta\varepsilon}{2}\cos\omega_0 t_1(\varepsilon\sin\omega_0\tau + gT\cos\omega_0\tau) \end{aligned} \tag{8}$$

At moderate times only slowly oscillating terms survive. They are the ones that involve $\Delta t = t_2 - 2t_1$. For the total work $W = W_1 + W_2$ the averaging over ω_0 brings

$$\begin{aligned} W &= \frac{g\hbar\Gamma}{\pi} - \frac{\hbar}{4}e^{-t_2/\mathcal{T}_2}e^{-|\Delta t|/\mathcal{T}_2^*}\tanh\frac{\beta\hbar\bar{\omega}_0}{2}\times \\ &\left\{\bar{\omega}_0\sin\bar{\omega}_0\Delta t + [\frac{1}{\mathcal{T}_2} - \frac{\mathrm{sg}(\Delta t)}{\mathcal{T}_2^*}(1+\frac{\beta\hbar\bar{\omega}_0}{\sinh\beta\hbar\bar{\omega}_0})]\cos\bar{\omega}_0\Delta t\right\} \end{aligned} \tag{9}$$

For Δt near $2\pi n/\bar{\omega}_0$ such that the odd terms cancel, this again exhibits work extracted solely from the bath.

Feasibility. Let us present several reasons favoring the feasibility of the proposed setups: 1) Two-level systems are widespread, because many quantum system act as two-level systems under proper conditions; 2) Detection in these systems is relatively easy, since already one-time quantities $\langle\vec{\sigma}(t)\rangle$ completely determine the state; 3) The harmonic oscillator bath is universal [11]; 4) Work and heat were measured in NMR experiments more than 35 years ago [12]; 5) Our main effects do survive the averaging over disordered ensembles of spins, thus allowing many-spin measurements. 6) The ongoing activity for implementation of quantum computers provides experimentally realized examples of two-level systems, which have sufficiently long $\mathcal{T}_2$ times, and

admit external variations on times smaller than $\mathscr{T}_2$: (*i*) for atoms in optical traps $\mathscr{T}_2 \sim 1$s, $1/\Gamma \sim 10^{-8}$s, and there are efficient methods for creating non-equilibrium initial states and manipulating atoms by external laser pulses [13]; (*ii*) for an electronic spin injected or optically excited in a semiconductor $\mathscr{T}_2 \sim 1\,\mu$s [14]; (*iii*) for an exciton created in a quantum dot $\mathscr{T}_2 \sim 10^{-9}$s [15] (in cases (*ii*) and (*iii*) $1/\Gamma \sim 10^{-13}$s and femtosecond (10^{-15}s) laser pulses are available); (*iv*) in NMR physics $\mathscr{T}_2 \sim 10^{-6} - 1$ s and the duration of pulses can be comparable with $1/\Gamma \sim 1\,\mu$s.

In conclusion, we have analyzed for the spin-boson model the validity of some non-equilibrium formulations of the second law. The model is relevant for almost any branch of condensed matter, where two-level systems are described: NMR and ESR [9], Josephson junctions [7], quantum optics [10]. Our main finding is that quantum coherence puts definite limits on the validity of non-equilibrium Thomson's formulation of the second law and on the validity of Clausius inequality. The effects disappear in the classical limit. The detailed discussion on the feasibility of the obtained effects can be found in [9].

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